Our current understanding of the microscopic origin of gradient terms

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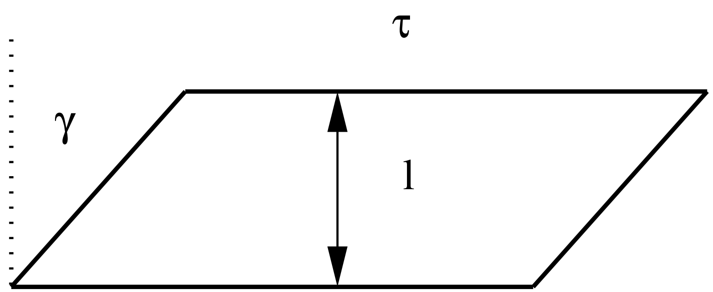
Outline

- Motivations
- Linking micro to meso-scale
- Properties of the correlation functions
- Gradient term
- Numerical results
- Extension for multiple slip
- Conclusions

Motivations



Local plasticity

$$\tau_{class}(\gamma, \dot{\gamma}, ...)$$

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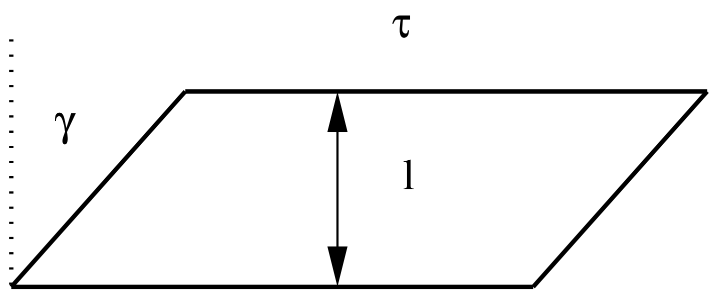

Local plasticity

$$\tau_{class}(\gamma, \dot{\gamma}, ...)$$

Phenomenological nonlocal plasticity

$$\tau(\gamma, \dot{\gamma}, ...) = \tau_{class}(\gamma, \dot{\gamma}, ...) + l^2 \mu \frac{d^2}{d\vec{r}^2} \gamma$$

Earlier examples

Fluid dynamics, Boltzmann equation

$$\frac{\partial}{\partial t} f + \vec{v}\frac{\partial}{\partial \vec{v}} f(t, \vec{v}, \vec{r}) + \vec{F}(\vec{r})\frac{\partial}{\partial \vec{r}} f(t, \vec{v}, \vec{r}) = \frac{\delta f_c}{\delta t}$$

$$\Downarrow$$

$$Navier - Stokes\ Equations$$

Plasma physics

$$BBGKY\ hierarhy$$

$$\Downarrow$$

$$Vlasov'sEquation$$

2D dislocation dynamics.

Equation of motion

$$\vec{v}_i = B\vec{b}\left(\sum_{j\neq i}^{N}\tau_{\text{ind}}(\vec{r}_i-\vec{r}_j)+\tau_{\text{ext}}\right), \quad \tau_{ind}(\vec{r}) = \frac{b\mu}{2\pi(1-\nu)}\frac{x(x^2-y^2)}{(x^2+y^2)^2}$$

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N particle density function

$$f_N(t, \vec{r}_1, \vec{r}_2 ... \vec{r}_N)d\vec{r}_1 d\vec{r}_2 ... d\vec{r}_N = f_N(t+\Delta t, \vec{r}'_1, \vec{r}'_2 ... \vec{r}'_N)d\vec{r}'_1 d\vec{r}'_2 ... d\vec{r}'_N$$
$$\vec{r}'_i = \vec{r}_i + \vec{v}_i \Delta t \qquad d\vec{r}'_i = d\vec{r}_i(1 + dv^i_x/dx_i \Delta t)$$

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$$\vec{r}\,'_i = \vec{r}_i + \vec{v}_i \Delta t \qquad d\vec{r}\,'_i = d\vec{r}_i (1 + dv_x^i / dx_i \Delta t)$$

From this

$$\frac{\partial f_N}{\partial t} + \sum_{i=1}^{N} \frac{\partial}{\partial \vec{r}_i} \{ f_N(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) \vec{v}_i \} = 0.$$

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$$\vec{r}\,'_i = \vec{r}_i + \vec{v}_i\Delta t \qquad d\vec{r}\,'_i = d\vec{r}_i(1 + dv^i_x/dx_i\Delta t)$$

With integration

$$\frac{\partial\rho_1(\vec{r}_1,t)}{\partial t} + \vec{b}\frac{d}{d\vec{r}_1}\left[\rho_1(\vec{r}_1,t)\tau_{\text{ext}} + \int \rho_2(\vec{r}_1,\vec{r}_2,t)\tau_{\text{ind}}(\vec{r}_1-\vec{r}_2)\mathrm{d}\vec{r}_2\right] = 0$$

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For dislocations with $\pm$ Burgers vectors

$$\frac{\partial\rho_+(\vec{r}_1,t)}{\partial t} + \vec{b}\frac{d}{d\vec{r}_1}\left[\rho_+(\vec{r}_1,t)\tau_{\mathrm{ext}} + \int\{\rho_{++}(\vec{r}_1,\vec{r}_2,t) - \rho_{+-}(\vec{r}_1,\vec{r}_2,t)\}\,\tau_{\mathrm{ind}}(\vec{r}_1-\vec{r}_2)\mathrm{d}\vec{r}_2\right] = 0$$

$$\frac{\partial\rho_-(\vec{r}_1,t)}{\partial t} - \vec{b}\frac{d}{d\vec{r}_1}\left[\rho_-(\vec{r}_1,t)\tau_{\mathrm{ext}} - \int\{\rho_{--}(\vec{r}_1,\vec{r}_2,t) - \rho_{-+}(\vec{r}_1,\vec{r}_2,t)\}\,\tau_{\mathrm{ind}}(\vec{r}_1-\vec{r}_2)\mathrm{d}\vec{r}_2\right] = 0$$

Long range $\Leftrightarrow$ Short range

Let

$$\rho_{ss'}(\vec{r}_1, \vec{r}_2, t) = \rho_s(\vec{r}_1)\rho_{s'}(\vec{r}_2)(1 + d_{ss'}(\vec{r}_1, \vec{r}_2)) \qquad s, s' \in \{+, -\}$$

Long range $\Leftrightarrow$ *Short range*

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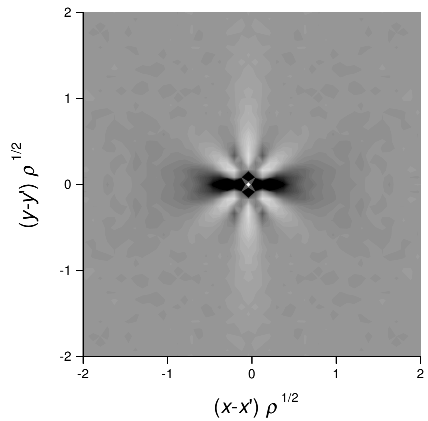

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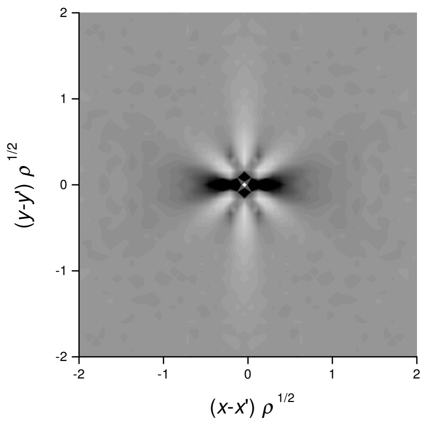
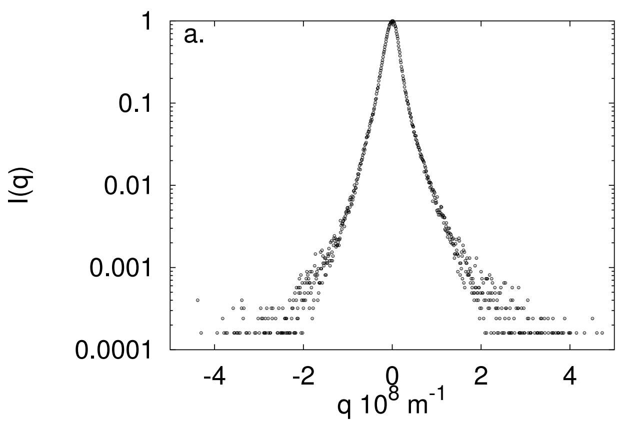


X ray line profile analysis



$$A(n) = \exp[\rho n^2 \ln(n/R)] \quad \sqrt{\rho}R \approx 1$$

Structure of equations

With $\rho = \rho_+ + \rho_-$ and $\kappa = \rho_+ - \rho_-$

$$\begin{aligned}
\frac{\partial \rho(\vec{r},t)}{\partial t} + \vec{b}\frac{d}{d\vec{r}}[\kappa(\vec{r},t)\,\{\tau_{\mathrm{sc}}(\vec{r}) + \tau_{\mathrm{ext}} - \tau_{\mathrm{f}}(\vec{r}) + \tau_{\mathrm{b}}(\vec{r})\}] &= f(\rho, \tau_{\mathrm{ext}}, \ldots) \\
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$$\tau_{\rm sc}(\vec{r}) = \int \kappa(\vec{r}_1, t)\tau_{\rm ind}(\vec{r} - \vec{r}_1)\mathrm{d}\vec{r}_1, \qquad \tau_{\rm ind} = \frac{x(x^2-y^2)}{(x^2+y^2)^2}$$

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Field equations (Kröner)

$$\Delta^2 \chi = -Ab\frac{\partial \kappa}{\partial y}, \quad \tau_{\mathrm{sc}} = \frac{\partial^2}{\partial x \partial y}\chi$$

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\tau_{\mathrm{b}}(\vec{r}) &= \int \kappa(\vec{r}_1) d(\vec{r} - \vec{r}_1)\tau_{\mathrm{ind}}(\vec{r} - \vec{r}_1)\mathrm{d}\vec{r_1} \qquad d = d_{+-} + d_{-+} + d_{++} + d_{--}
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\tau_{\rm b}(\vec{r}) &= -\frac{d\kappa(\vec{r})}{d\vec{r}}\int \vec{r}d(\vec{r})\tau_{\rm ind}(\vec{r}){\rm d}\vec{r}
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$$\begin{aligned}
\tau_{\rm f}(\vec{r}) &= \frac{\mu b}{2\pi(1-\nu)}C(\tau)\sqrt{\rho(\vec{r})} \\
\tau_{\rm b}(\vec{r}) &= -\frac{\mu b}{2\pi(1-\nu)}D\frac{1}{\rho(\vec{r})}\frac{\partial \kappa(\vec{r})}{\partial x}
\end{aligned}$$

Plasticity

By definition

$$b\kappa = -\frac{\partial \gamma}{\partial x}$$

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Rate of deformation

$$\dot{\gamma} = \kappa \left[\tau - \tau_{\mathrm{f}} - \frac{\mu b}{2\pi(1-\nu)} D \frac{1}{\rho(\vec{r})} \frac{\partial \kappa(\vec{r})}{\partial x} \right]$$

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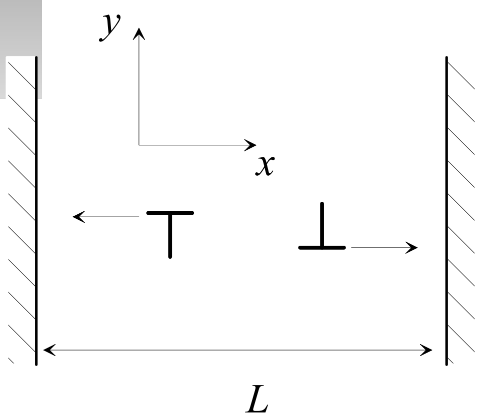
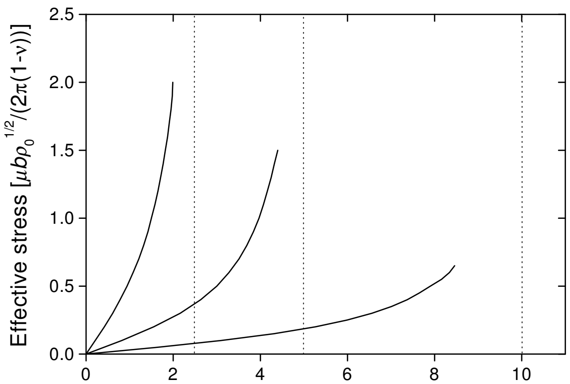
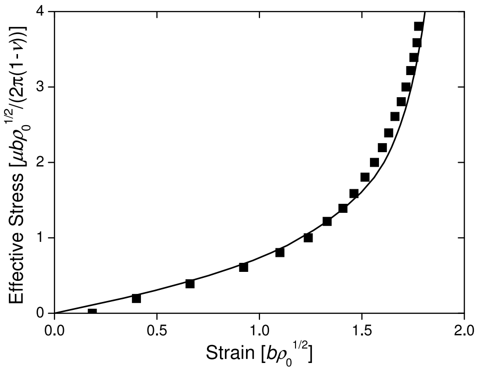
Gradient term

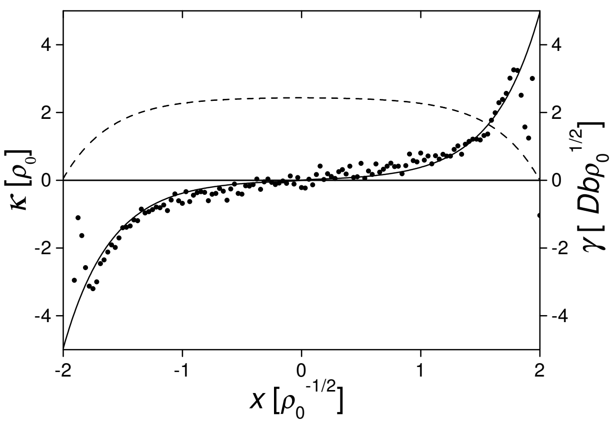
$$\tau_{eff} = \tau + \frac{\mu}{2\pi(1-\nu)}D\frac{1}{\rho(\vec{r})}\frac{\partial^2\gamma(\vec{r})}{\partial x^2}$$

Finite size effect









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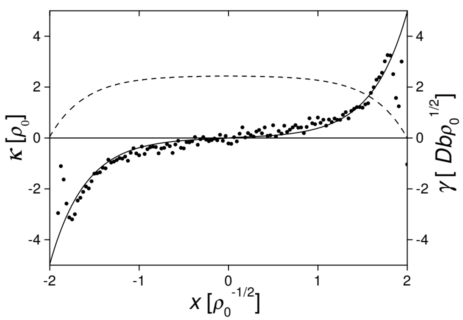

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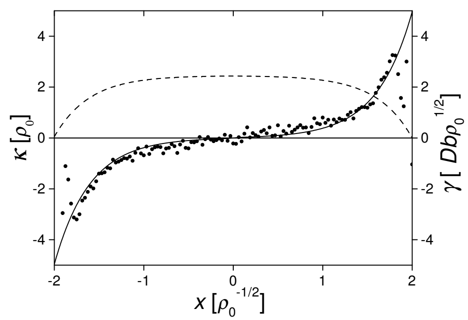
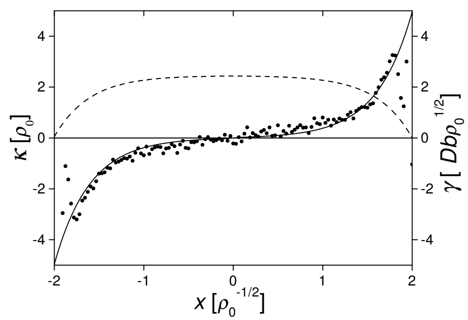


if $\rho = 1/l^2$

$$\tau = \frac{\mu b}{2\pi(1-\nu)} D \frac{1}{\rho(\vec{r})} \frac{\partial \kappa(\vec{r})}{\partial x}$$

$$\kappa(\vec{r}) = \tau \frac{1}{l^2} \frac{2\pi(1-\nu)}{\mu b D} x$$

Finite size effect



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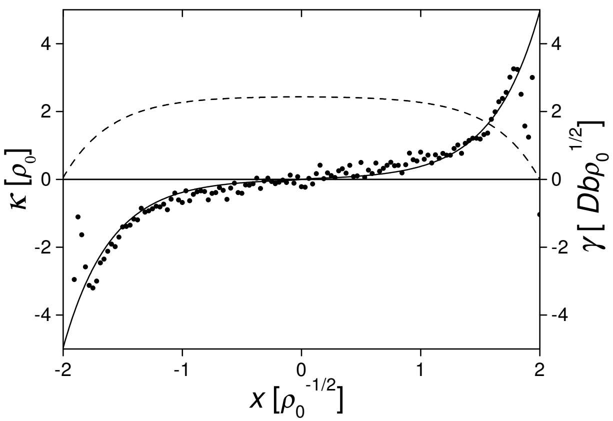
$$\kappa(\vec{r}) = \tau \frac{1}{l^2} \frac{2\pi(1-\nu)}{\mu b D} x$$

at the boundary $-L/2\ \rho = -\kappa$

$$\tau = -\frac{\mu b}{2\pi(1-\nu)} D \frac{1}{\kappa(\vec{r})} \frac{\partial \kappa(\vec{r})}{\partial x}$$

$$\kappa(\vec{r}) = \kappa_0 \exp\left\{ -\tau \frac{2\pi(1-\nu)}{\mu b D} x \right\}$$

Boundary layer



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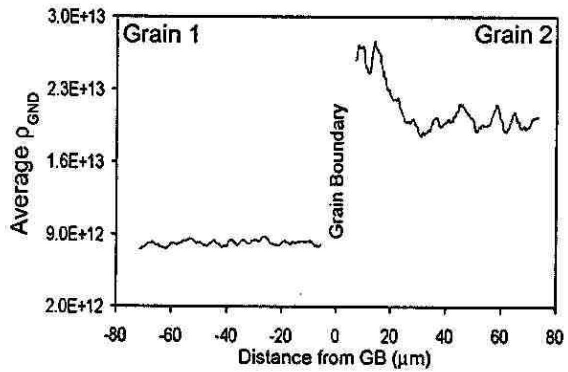
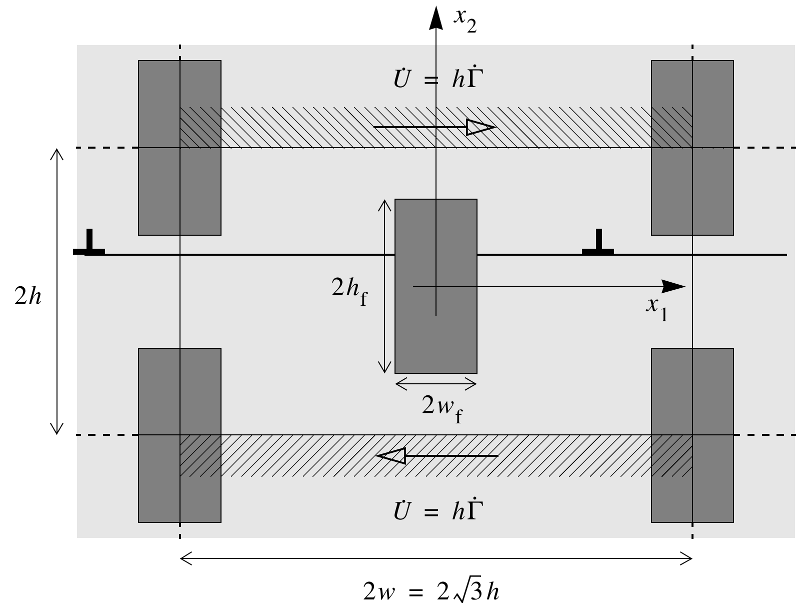


Fig. 3. Plot of the average ρ_{GND} as a function of the distance from the grain boundary.

Nontrivial problems (Erik, Serge)



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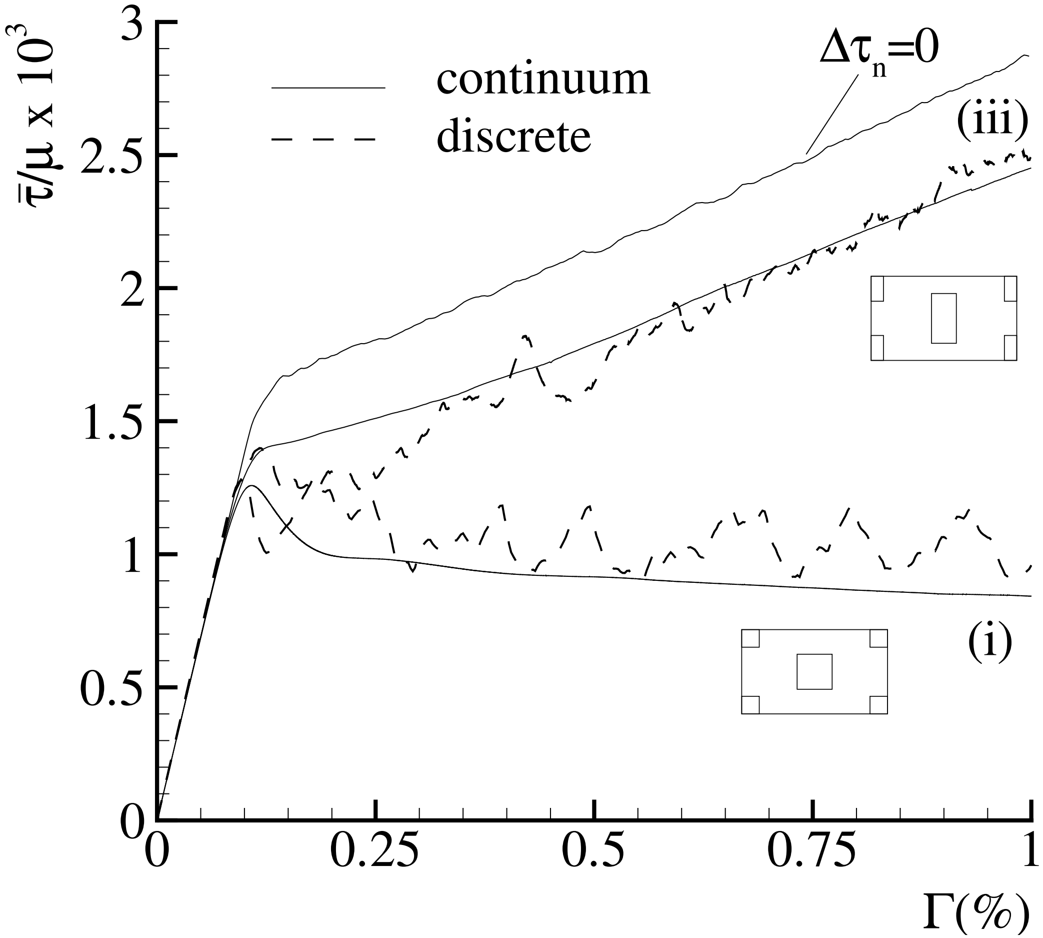

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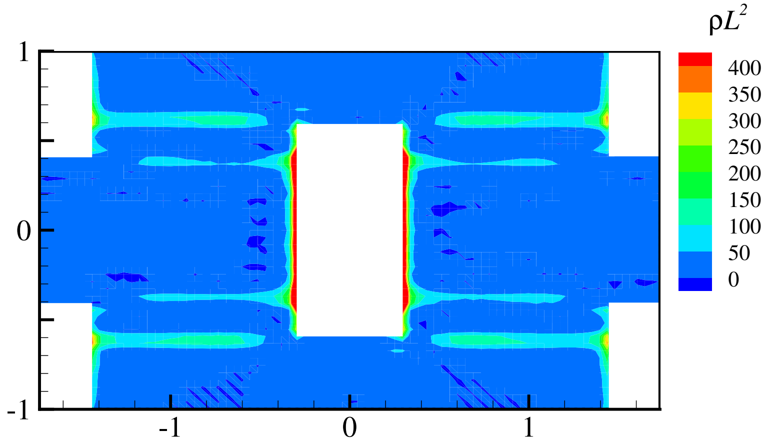
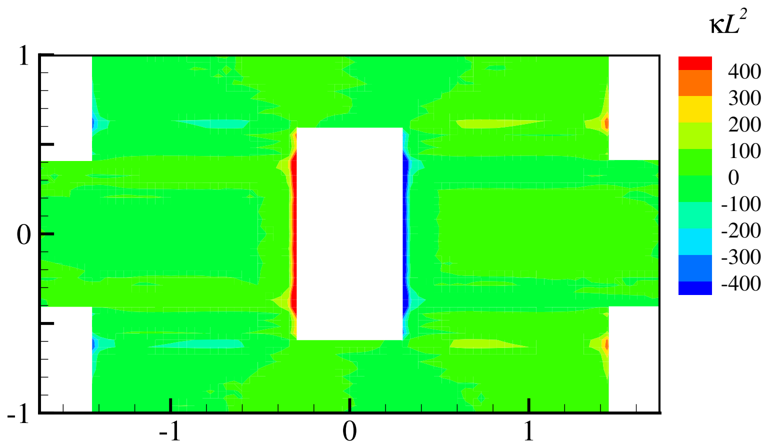




Multiple slip?

$$\frac{\partial \rho_i(\vec{r},t)}{\partial t} + \vec{b}_i \frac{d}{d\vec{r}}[\kappa_i(\vec{r},t)\left\{\tau_{\mathrm{sc}}(\vec{r}) + \tau^i_{\mathrm{ext}} - \tau^i_{\mathrm{f}}(\vec{r}) + \tau^i_{\mathrm{b}}(\vec{r})\right\}] = f_i(\rho_i, \tau^i_{\mathrm{ext}}, \dots)$$

$$\frac{\partial \kappa_i(\vec{r},t)}{\partial t} + \vec{b}_i \frac{d}{d\vec{r}}[\rho_i(\vec{r},t)\left\{\tau^i_{\mathrm{sc}}(\vec{r}) + \tau^i_{\mathrm{ext}} - \tau^i_{\mathrm{f}}(\vec{r}) + \tau^i_{\mathrm{b}}(\vec{r})\right\}] = 0,$$

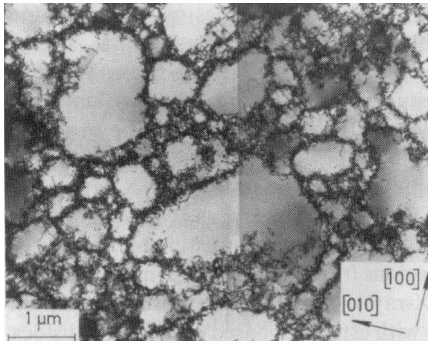
$$\tau^i_{\mathrm{b}}(\vec{r}) = -\sum_{j=1}^{N} D_{ij}(\rho_k)\vec{b}_j \frac{d\kappa_j(\vec{r})}{d\vec{r}}$$

Multiple slip?

$$\frac{\partial \rho_i(\vec{r},t)}{\partial t} + \vec{b}_i \frac{d}{d\vec{r}}[\kappa_i(\vec{r},t)\left\{\tau_{\mathrm{sc}}(\vec{r}) + \tau^i_{\mathrm{ext}} - \tau^i_{\mathrm{f}}(\vec{r}) + \tau^i_{\mathrm{b}}(\vec{r})\right\}] \quad = \quad f_i(\rho_i, \tau^i_{\mathrm{ext}}, \ldots)$$

$$\frac{\partial \kappa_i(\vec{r},t)}{\partial t} + \vec{b}_i \frac{d}{d\vec{r}}[\rho_i(\vec{r},t)\left\{\tau^i_{\mathrm{sc}}(\vec{r}) + \tau^i_{\mathrm{ext}} - \tau^i_{\mathrm{f}}(\vec{r}) + \tau^i_{\mathrm{b}}(\vec{r})\right\}] \quad = \quad 0,$$

$$\tau^i_{\mathrm{b}}(\vec{r}) \quad = \quad -\sum_{j=1}^{N} D_{ij}(\rho_k)\vec{b}_j \frac{d\kappa_j(\vec{r})}{d\vec{r}}$$



$$D_{ij}(\rho_k, \gamma)$$

Temperature?, Climb?

Temperature

$$v_x^i = B_g(T) b\tau(x_i, y_i) + \sqrt{kTB_g}\zeta_x^i \quad < \zeta_x^i(t)\zeta_x^i(0) >= \delta(t)$$

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Climb

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Fokker-Planck type equation

$$\frac{\partial}{\partial t}\rho_\pm \mp \frac{d}{d\vec{r}}\rho_\pm \hat{B}\frac{d}{d\vec{r}}V(\vec{r}) \mp \frac{d}{d\vec{r}}\hat{D}\frac{d}{d\vec{r}}(\rho_+ - \rho_-) + kT\frac{d}{d\vec{r}}\hat{B}\frac{d}{d\vec{r}}\rho_\pm = f(\rho_\pm, \ldots)$$

Summary

Continuum theory of dislocation dynamics

- Balance equation for ρ and κ
- Self-consistent (long range) field
- Flow stress
- Back stress, gradient term